

Protein Structural Variation in Computational Models and Crystallographic Data

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DOI 10.1016/j.str.2007.05.001

(Structure 15, 169–177; February 14, 2007)

An incorrect expression was shown for the measure of overlap of two ellipsoidal distributions. We used a modified version of the Merritt overlap score, which should replace the equation for $cc(U, V)$ on p. 176:

$$cc_{mod}(U, V) = \frac{cc(U, V) - cc(U^*, V^*)}{1 - cc(U^*, V^*)}, \quad (1)$$

where $cc(U, V)$ is the Merritt overlap score for normalized ellipsoids U and V , and $cc(U^*, V^*)$ is the overlap score for the same ellipsoids with the major axis aligned to the minor, giving the lowest possible overlap score. This modification was designed to give greater range for directional comparison, with 0 indicating perfect misalignment and 1, perfect alignment. The authors are grateful to Konrad Hinsén for bringing the error to our attention.